

Conditional stochastic averaging of steady state unsaturated flow by means of Kirchhoff transformation

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Abstract. We consider the effect of measuring randomly varying soil hydraulic properties on one's ability to predict steady state unsaturated flow subject to random sources and/or initial and boundary conditions. Our aim is to allow optimum unbiased prediction of system states (pressure head, water content) and fluxes deterministically, without upscaling and without linearizing the constitutive characteristics of the soil. It has been shown by *Neuman et al.* [1999] that such prediction is possible by means of first ensemble moments of system states and fluxes, conditioned on measured values of soil properties, when the latter scale in a linearly separable fashion as proposed by *Vogel et al.* [1991]; the uncertainty associated with such predictions can be quantified by means of the corresponding conditional second moments. The derivation of moment equations for soils whose properties do not scale in the above manner requires linearizing the corresponding constitutive relations, which may lead to major inaccuracies when these relations are highly nonlinear, as is often the case in nature. When the scaling parameter of pressure head is a random variable independent of location, the steady state unsaturated flow equation can be linearized by means of the Kirchhoff transformation for gravity-free flow. Linearization is also possible in the presence of gravity when hydraulic conductivity varies exponentially with pressure head. For the latter case we develop exact conditional first- and second-moment equations which are nonlocal and therefore non-Darcian. We solve these equations analytically by perturbation for unconditional vertical infiltration and compare our solution with the results of numerical Monte Carlo simulations. Our analytical solution demonstrates in a rigorous manner that the concept of effective hydraulic conductivity does not apply to ensemble-averaged unsaturated flow except when gravity is the sole driving force.

1. Introduction

Soil hydraulic parameters such as saturated hydraulic conductivity and porosity, water retention characteristics, and relative hydraulic conductivity have been traditionally viewed as well-defined local quantities that can be assigned unique values at each point in space. Yet subsurface flow takes place in a complex soil environment whose makeup varies in a manner that cannot be predicted deterministically in all of its relevant details. This makeup tends to exhibit discrete and continuous variations on a multiplicity of scales, causing hydraulic parameters to do likewise. In practice, such parameters can at best be measured at selected locations and depth intervals where their values depend on the scale (support volume) and mode (instrumentation and procedure) of measurement. Estimating the parameters at points where measurements are not available entails a random error. Quite often, the support of measurement is uncertain, and the data are corrupted by experimental and interpretive errors. These errors and uncertainties render the parameters random and the corresponding flow equation stochastic.

Though the uncertain nature of flow parameters is now widely recognized, there does not yet appear to be a consensus about the best way to deal with it mathematically. The most prevalent approach has been that represented by the geostatistical school of thought. According to this philosophy, parameter values determined at various points within a more or less distinct soil unit can be viewed as a sample from a random field defined over a continuum. This random field is characterized by a joint (multivariate) probability density function or, equivalently, its joint ensemble moments. Thus a parameter such as (saturated, natural) log hydraulic conductivity $Y(\mathbf{x}) = \ln K_s(\mathbf{x})$ varies not only across the real space coordinates \mathbf{x} within the unit, but also in probability space (this variation may be represented by another "coordinate" ξ which, for simplicity, we suppress). Whereas spatial moments are obtained by sampling $Y(\mathbf{x})$ in real space (across \mathbf{x}), ensemble moments are defined in terms of samples collected in probability space (across ξ).

If the statistical properties of $Y(\mathbf{x})$ and other relevant random parameters can be inferred from measurements, the stochastic flow equation can be solved numerically by (conditional) Monte Carlo simulation and the results analyzed statistically. The statistics most commonly computed from such simulations include (sample conditional) mean hydraulic (pressure) heads and gradients, saturations and/or water contents, relative hy-

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draulic conductivities, volumetric water fluxes, and seepage velocities. The true counterparts of these sample means constitute optimum (unbiased) predictors of system behavior under uncertainty. Another statistic commonly computed from Monte Carlo simulations is the (sample conditional) variance, and perhaps covariance, of the associated prediction errors.

The Monte Carlo approach is conceptually straightforward and has the advantage of applying to a very broad range of both linear and nonlinear flow and transport problems. It, however, has a number of potential drawbacks. To properly resolve high-frequency space-time fluctuations in the random parameters (including random initial and forcing terms), it is necessary to employ fine numerical grids in space-time. To avoid artificial boundary effects, these grids must span large space-time domains. Each sample calculation may therefore place a heavy demand on computer time and storage, especially when one deals with two- and three-dimensional nonlinear (unsaturated) flow in strongly heterogeneous media (where the discretized governing equation may become stiff). To insure that the sample output moments converge to their (generally unknown) theoretical ensemble values, a very large number of Monte Carlo runs is often required. Even if some sample moments appear to stabilize after a sufficiently large number of runs, there is generally no guarantee that they have in fact converged.

One alternative to Monte Carlo simulation is to use traditional deterministic models. However, since system outputs are generally nonlinear in the controlling parameters, the conditional mean outputs of Monte Carlo simulations are generally different from outputs one would obtain upon simply replacing the parameters in standard deterministic models by their (conditional) mean values. Such deterministic outputs would generally be biased and therefore less than optimal. To render deterministic models less biased, there has been an intensive search in the literature for "effective" or "equivalent" parameters that could be used to replace their suboptimal counterparts. The search has focused in large part on methods of "upscaling" which ascribe equivalent parameters to the grid blocks of numerical flow models on the basis of smaller-scale random (or nonrandom) parameter values. Traditionally, upscaling has been conducted numerically based on more or less ad hoc criteria of equivalence. More rigorous theoretical criteria of equivalence have been proposed for saturated hydraulic conductivity by *Indelman and Dagan* [1993], but these are not easy to implement in practice. Recent contributions to the upscaling of unsaturated flow properties include the works of *Bagtzoglou et al.* [1994] and *Desbarats* [1995].

A major conceptual difficulty with upscaling is that it postulates a local relationship between (conditional) mean driving force and flux (Darcy's law) when in fact this relationship is generally nonlocal [*Neuman and Orr*, 1993; *Neuman et al.*, 1996; *Tartakovsky and Neuman*, 1998a, b]. Even where localization is possible, the constitutive equations satisfied by conditional mean predictors may be fundamentally different from those satisfied by their random counterparts [*Neuman et al.*, 1999]. Another conceptual difficulty with traditional upscaling is that it requires the a priori definition of a numerical grid even though there are no firm theoretical guidelines for its selection. Hence it is necessary to continue developing alternative ways of predicting flow and transport deterministically in a manner consistent with (conditional) stochastic theory.

In this paper we present a deterministic alternative to (conditional) Monte Carlo simulation which allows predicting

steady state unsaturated flow under uncertainty, and assess the latter by means of conditional second moments, without having to generate random fields or variables, without upscaling, and without linearizing the constitutive characteristics of the soil. It has been shown by *Neuman et al.* [1999] that such prediction is possible by means of first ensemble moments of system states and fluxes, conditioned on measured values of soil properties, when the latter scale in a linearly separable fashion as proposed by *Vogel et al.* [1991]. This scaling differs from that of *Miller and Miller* [1956] or *Warrick et al.* [1977] in that it does not assume similarity of pore space geometries. It has been used by *Vogel et al.* to greatly reduce the scatter of pressure head versus water content data from 36 undisturbed 100 cm³ cores of clayey loam soil taken along a 500 m transect in the Trebon region of southern Bohemia, the Czech Republic; by *Neuman and Loeven* [1994] to do the same for pressure head versus saturation data from rock cores of Bandelier Tuff, extracted from depths of about 10–170 feet (3.0–51.8 m) in Los Alamos County, New Mexico; and by *Neuman et al.* [1999] to significantly reduce the scatter of water retention data from 497 soil samples at the Las Cruces trench experimental site in New Mexico [*Wierenga et al.*, 1989, 1991]. *Neuman et al.* have shown that in the particular case where the scaling parameter of pressure head is a random variable independent of location, the steady state unsaturated flow equation can be linearized by means of the Kirchhoff transformation for gravity-free flow. Linearization is also possible in the presence of gravity when hydraulic conductivity varies exponentially with pressure head according to the model of *Gardner* [1958].

The derivation of moment equations for soils whose properties do not scale in the above manner requires linearizing the corresponding constitutive relations. This may lead to major inaccuracies when these relations are highly nonlinear, as is often the case in nature. Virtually all previously published moment analyses of unsaturated flow, whether analytical [*Andersson and Shapiro*, 1983; *Yeh et al.*, 1985a, b; *Mantoglou and Gelhar*, 1987; *Yeh*, 1989; *Mantoglou*, 1992; *Russo*, 1995; *Zhang et al.*, 1998] or numerical [*Zhang and Winter*, 1998], have found it necessary to rely on perturbative approximations of soil constitutive relations. A major purpose of our paper is to show how one can preserve the nonlinear nature of *Gardner's* [1958] exponential relationship between hydraulic conductivity and pressure head in a stochastic moment analysis of steady state flow under gravity, by using the Kirchhoff transformation. This requires that we treat the exponent α in this relationship as a random constant rather than a spatially varying random field. Though this is an important limitation, we feel that it is a relatively small price to pay for the advantage of preserving constitutive nonlinearity. We explore the extent to which our assumptions regarding the properties of α are justified by providing a brief review of published studies concerning its spatial variability. Treating it as a random constant allows us to develop exact conditional first- and second-moment equations for steady state unsaturated flow which have integrodifferential forms similar to those developed for steady state saturated flow by *Neuman and Orr* [1993], *Neuman et al.* [1996], and *Guadagnini and Neuman* [1997, 1998]. Upon introducing the additional assumption that α has a relatively small variance, the Kirchhoff transformation allows us to solve these stochastic moment equations analytically by perturbation in terms of a small parameter representing the variance of the natural logarithm of saturated hydraulic conductivity. We do so for unconditional vertical infiltration and compare our solution with

the results of numerical Monte Carlo simulations. Our analytical solution demonstrates in a rigorous manner that the concept of effective hydraulic conductivity does not apply to stochastically averaged unsaturated flow except when gravity is the sole driving force.

2. Statement of the Problem

Following Russo [1992] and Neuman and Orr [1993], we start from the premise that Darcy's law

$$\mathbf{q}(\mathbf{x}) = -K(\mathbf{x}, \psi) \nabla[\psi(\mathbf{x}) + x_3] \quad (1)$$

applies when the flux $\mathbf{q}(\mathbf{x})$, the unsaturated hydraulic conductivity $K(\mathbf{x}, \psi)$, and the gradient $\nabla\psi(\mathbf{x})$ of pressure head are representative of a support (measurement) volume ω centered about the point $\mathbf{x} = (x_1, x_2, x_3)^T$ where x_3 is the vertical coordinate (taken to be positive upward).

Consider steady state flow in a heterogeneous soil within the flow domain Ω which is large in comparison to the support ω and is bounded by a surface Γ . Flow is governed by the continuity equation

$$-\nabla \cdot \mathbf{q}(\mathbf{x}) + f(\mathbf{x}) = 0 \quad \mathbf{x} \in \Omega \quad (2)$$

subject to the boundary conditions

$$\psi(\mathbf{x}) = \Psi(\mathbf{x}) \quad \mathbf{x} \in \Gamma_D \quad (3)$$

$$-\mathbf{q}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) = Q(\mathbf{x}) \quad \mathbf{x} \in \Gamma_N. \quad (4)$$

Here $f(\mathbf{x})$ is a randomly prescribed source function, $\Psi(\mathbf{x})$ is a randomly prescribed pressure head on Dirichlet boundary segments Γ_D , $Q(\mathbf{x})$ is randomly prescribed flux across Neumann boundary segments Γ_N , $\mathbf{n} = (n_1, n_2, n_3)^T$ is a unit outward normal to the boundary Γ , and $\Gamma = \Gamma_D \cup \Gamma_N$. Though it is not strictly necessary, we assume for simplicity that the source and boundary functions $f(\mathbf{x})$, $\Psi(\mathbf{x})$, and $Q(\mathbf{x})$ are prescribed in a statistically independent manner.

We take the constitutive relationship $K(\mathbf{x}, \psi)$ to be given by the exponential model [Gardner, 1958]

$$K(\mathbf{x}, \psi) = K_s(\mathbf{x}) K_r(\mathbf{x}, \psi) \quad K_r(\mathbf{x}, \psi) = e^{\alpha(\mathbf{x})\psi} \quad (5)$$

where K_s and K_r are saturated and relative hydraulic conductivity, respectively, and α is the reciprocal of the macroscopic capillary length scale [Raats, 1976]. Spatial variations in the constitutive parameters K_s and α , coupled with a lack of detailed information about their spatial distributions, render K_s and α random. This and the uncertain forcing terms in (1)–(5) render these differential equations stochastic.

It is known that the Gardner model often fails to reproduce adequately measured relationships between K_r and ψ over the entire range of relevant saturations [Russo, 1988]; in this sense other models, such as those of van Genuchten [1978] or Brooks and Corey [1964] (see also Zhang and Winter [1998] and Zhang et al. [1998]) tend to do better. The Gardner model is nevertheless appealing due to its relative simplicity, which has made it a favorite among analysts of unsaturated flow in randomly heterogeneous soils. Whereas much is known about the spatial variability of K_s , relatively few studies have concerned themselves with the spatial statistics of α [Reynolds and Elrick, 1985; Greenholtz et al., 1988; White and Sully, 1987, 1992; Ünlü et al., 1990; Russo and Bouton, 1992; Ragab and Cooper, 1993a, b; Russo et al., 1997]. All but one of these studies found both K_s and α to be lognormally distributed; only Ünlü et al. [1990]

found α to be approximately normal. White and Sully [1992] attributed the lognormality of both K_s and α to the dependence of both parameters on the internal pore structure of the soil. Values of α appear to depend strongly on soil texture and vegetation: White and Sully [1987] found α to range from 0.05 cm^{-1} for clay to 0.71 cm^{-1} for gravely loam fine sand; Ragab and Cooper [1993a, b] reported ranges of 0.15–1.34 cm^{-1} for grassland, 0.36–0.37 cm^{-1} for woodland, and 0.28–0.89 cm^{-1} for arable land. The variance of $\ln \alpha$ can be either large or small relative to that of $\ln K_s$, depending on the study: Ünlü et al. [1990] reported variances of $\ln \alpha$ in the range 0.045–0.112, compared to a range of 0.391–0.960 for the variance of $\ln K_s$; Russo et al. [1997] found the variance of $\ln \alpha$ to be of the order of 0.425, compared to 1.242 for $\ln K_s$; according to Russo and Bouton [1992] and White and Sully [1992], the variances of $\ln \alpha$ and $\ln K_s$ are of similar orders; Ragab and Cooper [1993a, b] found the variance of $\ln \alpha$ to exceed that of $\ln K_s$. Both the latter authors and Russo [1992] reported large coefficients of variation for $\ln \alpha$.

Ragab and Cooper [1993a, b] had found a lack of cross correlation between $\ln \alpha$ and $\ln K_s$; in all three soil types they have investigated. Russo and Bouton [1992] treated $\ln \alpha$ and $\ln K_s$ as independent (and thus uncorrelated) random functions based on experimental evidence due to Russo [1983, 1984]. In their view, such lack of cross correlation is to be expected because in field soils, K_s is controlled by structural (macro-)voids, while α is controlled by the entire continuum of pore sizes. On the other hand, Russo et al. [1997] found $\ln \alpha$ and $\ln K_s$ data to exhibit a moderate correlation coefficient of 0.68, while Ünlü et al. [1990] reported a correlation coefficient as high as 0.80.

According to Russo and Bouton [1992] and Russo et al. [1997], the horizontal and vertical spatial autocorrelation scales of $\ln \alpha$ are about one-third the corresponding autocorrelation scales of $\ln K_s$. The $\ln \alpha$ data of Ünlü et al. [1990] exhibit a relatively large nugget variance and spatial autocorrelations scales larger than those of $\ln K_s$ values which, however, were based in part on linear regression rather than on direct measurement [Russo and Bouton, 1992, p. 1921].

Considering the above findings, we feel comfortable treating both K_s and α as being lognormally distributed. We also feel comfortable disregarding cross correlations between K_s and α , and their logarithms, as these correlations are weak in the majority of soils examined to date. Though our general theory allows α to have a variance of order comparable to that of K_s , our perturbation analyses have been limited for simplicity to soils in which the former is small compared to the latter and can therefore be disregarded. Our review makes clear that statistically homogeneous soils in which this is appropriate do exist. In such soils, disregarding the variance of α is tantamount to setting its values everywhere equal to a spatially uniform ensemble mean (expectation), as we do. Treating α as being spatially uniform when its variance, relative to that of K_s , is significant (as we allow in our general theory) requires that its spatial autocorrelation scales be relatively large. Available data suggest that this may be the case in some soils but not in others. As we have already stated, we are willing to pay the price of limiting the class of soils to which our theory applies, considering the rewards offered by its unique ability to fully preserve the nonlinearity of the associated constitutive relationship between relative hydraulic conductivity and pressure head. Precedents for treating α as being spatially uniform, in soils that

are otherwise heterogeneous, are provided by *Yeh et al.* [1985a] and *Weir* [1989].

3. Nonlocal Formalism

Substituting (1) into (2) yields the Richards equation

$$\nabla \cdot \{K_s(\mathbf{x}) K_r(\psi) \nabla [\psi(\mathbf{x}) + x_3]\} + f(\mathbf{x}) = 0 \quad \mathbf{x} \in \Omega. \quad (6)$$

Upon applying the Kirchhoff transformation [*Ames*, 1967]

$$\Phi(\mathbf{x}) = \int_{-\infty}^{\psi(\mathbf{x})} K_r(t) dt = \frac{1}{\alpha} e^{\alpha\psi}, \quad (7)$$

(6) becomes a linear partial differential equation [*Gardner*, 1958],

$$\nabla \cdot [K_s(\mathbf{x}) \nabla \Phi(\mathbf{x})] + \alpha \frac{\partial}{\partial x_3} [K_s(\mathbf{x}) \Phi(\mathbf{x})] + f(\mathbf{x}) = 0 \quad (8)$$

$$\mathbf{x} \in \Omega.$$

Transformation of the boundary conditions (3) and (4) yields

$$\Phi(\mathbf{x}) = H(\mathbf{x}) \quad H(\mathbf{x}) = \frac{1}{\alpha} e^{\alpha\psi} \quad \mathbf{x} \in \Gamma_D \quad (9)$$

$$K_s(\mathbf{x}) \nabla \Phi(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) + \alpha n_3(\mathbf{x}) K_s(\mathbf{x}) \Phi(\mathbf{x}) = Q(\mathbf{x}) \quad (10)$$

$$\mathbf{x} \in \Gamma_N.$$

We represent random fields and variables as sums of conditional means $\langle A \rangle_c$ and zero-mean perturbations A' about them,

$$K_s(\mathbf{x}) = \langle K_s(\mathbf{x}) \rangle_c + K'_s(\mathbf{x}) \quad \langle K'_s(\mathbf{x}) \rangle_c \equiv 0 \quad (11)$$

$$\alpha = \langle \alpha \rangle + \alpha' \quad \langle \alpha' \rangle \equiv 0 \quad (12)$$

$$\Phi(\mathbf{x}) = \langle \Phi(\mathbf{x}) \rangle_c + \Phi'(\mathbf{x}) \quad \langle \Phi'(\mathbf{x}) \rangle_c \equiv 0 \quad (13)$$

where the subscript c indicates conditioning on the same saturated hydraulic conductivity data used to obtain $\langle K_s(\mathbf{x}) \rangle_c$. Taking the conditional ensemble mean of (8)–(10) while treating α as a random constant gives

$$\nabla \cdot [\langle K_s(\mathbf{x}) \rangle_c \nabla \langle \Phi(\mathbf{x}) \rangle_c - \mathbf{r}_c(\mathbf{x})] + \frac{\partial}{\partial x_3} [\langle \alpha \rangle \langle K_s(\mathbf{x}) \rangle_c \langle \Phi(\mathbf{x}) \rangle_c + \langle \alpha \rangle \sigma_{K\Phi}^2(\mathbf{x}) + \langle K_s(\mathbf{x}) \rangle_c \sigma_{\alpha\Phi}^2(\mathbf{x}) + \langle \alpha' K'_s(\mathbf{x}) \Phi'(\mathbf{x}) \rangle_c] + \langle f(\mathbf{x}) \rangle = 0 \quad \mathbf{x} \in \Omega \quad (14)$$

$$\mathbf{r}_c(\mathbf{x}) = -\langle K'_s(\mathbf{x}) \nabla \Phi'(\mathbf{x}) \rangle_c \quad (15)$$

$$\sigma_{K\Phi}^2(\mathbf{x}) = \langle K'_s(\mathbf{x}) \Phi'(\mathbf{x}) \rangle_c \quad \sigma_{\alpha\Phi}^2(\mathbf{x}) = \langle \alpha' \Phi'(\mathbf{x}) \rangle_c$$

$$\langle \Phi(\mathbf{x}) \rangle_c = \langle H(\mathbf{x}) \rangle \quad \mathbf{x} \in \Gamma_D \quad (16)$$

$$\mathbf{n}(\mathbf{x}) \cdot [\langle K_s(\mathbf{x}) \rangle_c \nabla \langle \Phi(\mathbf{x}) \rangle_c - \mathbf{r}_c(\mathbf{x})] + n_3(\mathbf{x}) [\langle \alpha \rangle \cdot \langle K_s(\mathbf{x}) \rangle_c \langle \Phi(\mathbf{x}) \rangle_c + \langle \alpha \rangle \sigma_{K\Phi}^2(\mathbf{x}) + \langle K_s(\mathbf{x}) \rangle_c \sigma_{\alpha\Phi}^2(\mathbf{x}) + \langle \alpha' K'_s(\mathbf{x}) \Phi'(\mathbf{x}) \rangle_c] = \langle Q(\mathbf{x}) \rangle \quad \mathbf{x} \in \Gamma_N \quad (17)$$

where $\langle f(\mathbf{x}) \rangle$, $\langle H(\mathbf{x}) \rangle$, and $\langle Q(\mathbf{x}) \rangle$ are prescribed unconditional ensemble means of the statistically independent random forcing (source and boundary) functions $f(\mathbf{x})$, $H(\mathbf{x})$, and $Q(\mathbf{x})$, respectively.

In a manner similar to that followed by *Neuman et al.* [1996]

for saturated flow, we derive in Appendix A the following system of implicit equations for the “residual flux” $\mathbf{r}_c(\mathbf{x})$ and the conditional cross variances $\sigma_{K\Phi}^2(\mathbf{x})$ and $\sigma_{\alpha\Phi}^2(\mathbf{x})$:

$$\begin{aligned} \mathbf{r}_c(\mathbf{x}) = & \int_{\Omega} \tilde{\mathbf{a}}_c(\mathbf{x}, \mathbf{y}) \nabla_y \langle \Phi(\mathbf{y}) \rangle_c d\mathbf{y} + \int_{\Omega} \mathbf{a}_c(\mathbf{x}, \mathbf{y}) \langle \Phi(\mathbf{y}) \rangle_c d\mathbf{y} \\ & + \int_{\Omega} \tilde{\mathbf{b}}_c(\mathbf{x}, \mathbf{y}) \mathbf{r}_c(\mathbf{y}) d\mathbf{y} - \langle \alpha \rangle \int_{\Omega} \mathbf{b}_c(\mathbf{x}, \mathbf{y}) \sigma_{K\Phi}^2(\mathbf{y}) d\mathbf{y} \\ & - \int_{\Omega} \langle K_s(\mathbf{y}) \rangle_c \mathbf{b}_c(\mathbf{x}, \mathbf{y}) \sigma_{\alpha\Phi}^2(\mathbf{y}) d\mathbf{y} \\ & - \int_{\Omega} \left\langle K'_s(\mathbf{x}) \nabla_x \frac{\partial}{\partial y_3} \mathcal{G}(\mathbf{y}, \mathbf{x}) \right\rangle_c \langle \alpha' K'_s(\mathbf{y}) \Phi'(\mathbf{y}) \rangle_c d\mathbf{y} \end{aligned} \quad (18)$$

$$\begin{aligned} \sigma_{K\Phi}^2(\mathbf{x}) = & - \int_{\Omega} \mathbf{c}_c(\mathbf{x}, \mathbf{y}) \cdot \nabla_y \langle \Phi(\mathbf{y}) \rangle_c d\mathbf{y} \\ & - \int_{\Omega} \left[\langle \alpha \rangle c_{3c}(\mathbf{x}, \mathbf{y}) + \left\langle \alpha' K'_s(\mathbf{y}) \frac{\partial}{\partial y_3} \mathcal{G}(\mathbf{y}, \mathbf{x}) \right\rangle_c \right] \langle \Phi(\mathbf{y}) \rangle_c d\mathbf{y} \\ & - \int_{\Omega} \mathbf{d}_c(\mathbf{x}, \mathbf{y}) \cdot \mathbf{r}_c(\mathbf{y}) d\mathbf{y} + \langle \alpha \rangle \int_{\Omega} d_{3c}(\mathbf{x}, \mathbf{y}) \sigma_{K\Phi}^2(\mathbf{y}) d\mathbf{y} \\ & + \int_{\Omega} \langle K_s(\mathbf{y}) \rangle_c d_{3c}(\mathbf{x}, \mathbf{y}) \sigma_{\alpha\Phi}^2(\mathbf{y}) d\mathbf{y} \\ & + \int_{\Omega} d_{3c}(\mathbf{x}, \mathbf{y}) \langle \alpha' K'_s(\mathbf{y}) \Phi'(\mathbf{y}) \rangle_c d\mathbf{y}. \end{aligned} \quad (19)$$

The equation for $\sigma_{\alpha\Phi}^2(\mathbf{x})$ is obtained upon replacing $K'_s(\mathbf{x})$ in the kernels (22) of (19) by α' . Here $\tilde{\mathbf{a}}_c(\mathbf{x}, \mathbf{y})$ and $\tilde{\mathbf{b}}_c(\mathbf{x}, \mathbf{y})$ are second-rank tensors while $\mathbf{a}_c(\mathbf{x}, \mathbf{y})$, $\mathbf{b}_c(\mathbf{x}, \mathbf{y})$, $\mathbf{c}_c(\mathbf{x}, \mathbf{y}) = (c_{1c}, c_{2c}, c_{3c})^T$ and $\mathbf{d}_c(\mathbf{x}, \mathbf{y}) = (d_{1c}, d_{2c}, d_{3c})^T$ are vectors given formally by

$$\tilde{\mathbf{a}}_c(\mathbf{x}, \mathbf{y}) = \langle K'_s(\mathbf{x}) K'_s(\mathbf{y}) \nabla_x \nabla_y^T \mathcal{G}(\mathbf{y}, \mathbf{x}) \rangle_c \quad (20)$$

$$\tilde{\mathbf{b}}_c(\mathbf{x}, \mathbf{y}) = \langle K'_s(\mathbf{x}) \nabla_x \nabla_y^T \mathcal{G}(\mathbf{y}, \mathbf{x}) \rangle_c$$

$$\mathbf{a}_c(\mathbf{x}, \mathbf{y}) = \left\langle K'_s(\mathbf{x}) [\langle \alpha \rangle K'_s(\mathbf{y}) + \alpha' K'_s(\mathbf{y})] \nabla_x \frac{\partial}{\partial y_3} \mathcal{G}(\mathbf{y}, \mathbf{x}) \right\rangle_c \quad (21)$$

$$\mathbf{b}_c(\mathbf{x}, \mathbf{y}) = \left\langle K'_s(\mathbf{x}) \nabla_x \frac{\partial}{\partial y_3} \mathcal{G}(\mathbf{y}, \mathbf{x}) \right\rangle_c$$

$$\mathbf{c}_c(\mathbf{x}, \mathbf{y}) = \langle K'_s(\mathbf{x}) K'_s(\mathbf{y}) \nabla_y \mathcal{G}(\mathbf{y}, \mathbf{x}) \rangle_c \quad (22)$$

$$\mathbf{d}_c(\mathbf{x}, \mathbf{y}) = \langle K'_s(\mathbf{x}) \nabla_y \mathcal{G}(\mathbf{y}, \mathbf{x}) \rangle_c$$

where the random auxiliary function $\mathcal{G}(\mathbf{y}, \mathbf{x})$ satisfies the adjoint stochastic differential equation

$$\nabla_y \cdot [K_s(\mathbf{y}) \nabla_y \mathcal{G}(\mathbf{y}, \mathbf{x})] - \alpha K_s(\mathbf{y}) \frac{\partial}{\partial y_3} \mathcal{G}(\mathbf{y}, \mathbf{x}) + \delta(\mathbf{y} - \mathbf{x}) = 0 \quad \mathbf{y}, \mathbf{x} \in \Omega \quad (23)$$

subject to the homogeneous boundary conditions

$$\mathcal{G}(\mathbf{y}, \mathbf{x}) = 0 \quad \mathbf{y} \in \Gamma_D \quad (24)$$

$$\nabla \mathcal{G}(\mathbf{y}, \mathbf{x}) \cdot \mathbf{n}(\mathbf{y}) = 0 \quad \mathbf{y} \in \Gamma_N. \quad (25)$$

Evaluating the kernels (20)–(22) is problematic because they contain mixed moments of the random auxiliary function $\mathcal{G}(\mathbf{y}, \mathbf{x})$. To evaluate them, one would need to use either high-resolution (conditional) Monte Carlo simulation or adopt some type of closure approximation (such as the perturbation approximation we employ in the next section). This notwithstanding, the above results provide important insight into the fundamental properties of the kernels, most notably that they are nonlocal (i.e., depend on more than one point in space) and conditional on data (therefore nonunique).

As in the case of saturated flow [Neuman and Orr, 1993], it follows from the nonlocal nature of the residual flux $\mathbf{r}_c(\mathbf{x})$ and the conditional cross variances $\sigma_{K\Phi}^2(\mathbf{x})$ and $\sigma_{\alpha\Phi}^2(\mathbf{x})$ that $\langle K_s(\mathbf{x}) \rangle_c$, the best available unbiased estimate of the otherwise unknown random function $K_s(\mathbf{x})$, does not represent an effective saturated hydraulic conductivity in our deterministic formulation of the stochastic unsaturated flow problem. In fact, such an effective conductivity does not strictly exist unless $\mathbf{r}_c(\mathbf{x})$, $\sigma_{K\Phi}^2(\mathbf{x})$ and $\sigma_{\alpha\Phi}^2(\mathbf{x})$ are amenable to localization. It follows from (18)–(19) that in order for the conditional mean unsaturated flow equations (14)–(17) to become local, one must have

$$\langle \Phi(\mathbf{x}) \rangle_c \equiv \langle \Phi(\mathbf{x}) \rangle \equiv \Phi_0 = \text{const.} \quad (26)$$

By virtue of (7), this implies $\langle \psi(\mathbf{x}) \rangle \equiv \text{const}$ so that mean flow is controlled entirely by gravity. This explains why most, if not all, reported successes in upscaling unsaturated hydraulic conductivity $K(\mathbf{x}, \psi)$ [Yeh *et al.*, 1985a, b; Yeh, 1989; Russo, 1992] have dealt with downward flow under a unit mean hydraulic gradient.

4. Perturbation Analysis

To render the formal conditional mean flow equations (14)–(17) workable, we expand them in small parameters σ_Y and σ_β representing a measure of the standard deviation of $Y'(\mathbf{x}) = Y(\mathbf{x}) - \langle Y(\mathbf{x}) \rangle_c$ and $\beta' = \beta - \langle \beta \rangle$, respectively, where $Y(\mathbf{x}) = \ln K_s(\mathbf{x})$ and $\beta = \ln \alpha$. Experimental data reviewed earlier suggest that in the majority of soils, $\sigma_\beta^2 \ll \sigma_Y^2$. Upon restricting our analysis to such soils, we can simplify the analysis by considering only zeroth-order approximation in σ_β together with i th order approximations in σ_Y .

Expanding $\Phi(\mathbf{x})$, $K_s(\mathbf{x})$, and $\mathcal{G}(\mathbf{y}, \mathbf{x})$ in powers of $Y'(\mathbf{x})$ and collecting terms of like powers of σ_Y yields the zeroth-order approximation

$$\nabla \cdot [K_G(\mathbf{x}) \nabla \langle \Phi^{(0)}(\mathbf{x}) \rangle_c] + \langle \alpha \rangle \frac{\partial}{\partial x_3} [K_G(\mathbf{x}) \langle \Phi^{(0)}(\mathbf{x}) \rangle_c] + \langle f(\mathbf{x}) \rangle = 0 \quad \mathbf{x} \in \Omega \quad (27)$$

$$\langle \Phi^{(0)}(\mathbf{x}) \rangle_c = \langle H(\mathbf{x}) \rangle \quad \mathbf{x} \in \Gamma_D \quad (28)$$

$$K_G(\mathbf{x}) \mathbf{n}(\mathbf{x}) \cdot \nabla \langle \Phi^{(0)}(\mathbf{x}) \rangle_c + \langle \alpha \rangle n_3(\mathbf{x}) K_G(\mathbf{x}) \langle \Phi^{(0)}(\mathbf{x}) \rangle_c = \langle Q(\mathbf{x}) \rangle \quad \mathbf{x} \in \Gamma_N \quad (29)$$

and the second-order approximation (in σ_Y)

$$\begin{aligned} \nabla \cdot \left[K_G(\mathbf{x}) \nabla \langle \Phi^{(2)} \rangle_c + K_G(\mathbf{x}) \frac{\sigma_Y^2(\mathbf{x})}{2} \nabla \langle \Phi^{(0)}(\mathbf{x}) \rangle_c - \mathbf{r}_c^{(2)}(\mathbf{x}) \right] \\ + \langle \alpha \rangle \frac{\partial}{\partial x_3} \left[K_G(\mathbf{x}) \langle \Phi^{(2)} \rangle_c \right. \\ \left. + K_G(\mathbf{x}) \frac{\sigma_Y^2(\mathbf{x})}{2} \langle \Phi^{(0)}(\mathbf{x}) \rangle_c + \sigma_{K\Phi}^2(\mathbf{x}) \right] = 0 \end{aligned} \quad \mathbf{x} \in \Omega \quad (30)$$

$$\langle \Phi^{(2)}(\mathbf{x}) \rangle_c = 0 \quad \mathbf{x} \in \Gamma_D \quad (31)$$

$$\begin{aligned} \mathbf{n}(\mathbf{x}) \cdot \left[K_G(\mathbf{x}) \nabla \langle \Phi^{(2)} \rangle_c + K_G(\mathbf{x}) \frac{\sigma_Y^2(\mathbf{x})}{2} \nabla \langle \Phi^{(0)}(\mathbf{x}) \rangle_c - \mathbf{r}_c^{(2)}(\mathbf{x}) \right] \\ + \langle \alpha \rangle n_3(\mathbf{x}) \left[K_G(\mathbf{x}) \langle \Phi^{(2)} \rangle_c \right. \\ \left. + K_G(\mathbf{x}) \frac{\sigma_Y^2(\mathbf{x})}{2} \langle \Phi^{(0)}(\mathbf{x}) \rangle_c + \sigma_{K\Phi}^2(\mathbf{x}) \right] = 0 \end{aligned} \quad \mathbf{x} \in \Gamma_N \quad (32)$$

where $K_G = \exp(\langle Y \rangle)$ is the geometric mean of K_s . Second-order approximations of $\mathbf{r}_c(\mathbf{x})$ and $\sigma_{K\Phi}^2(\mathbf{x})$ are given by

$$\begin{aligned} \mathbf{r}_c^{(2)}(\mathbf{x}) = \int_{\Omega} \tilde{\mathbf{a}}_c^{(2)}(\mathbf{x}, \mathbf{y}) \nabla_{\mathbf{y}} \langle \Phi^{(0)}(\mathbf{y}) \rangle_c d\mathbf{y} \\ + \langle \alpha \rangle \int_{\Omega} \mathbf{a}_c^{(2)}(\mathbf{x}, \mathbf{y}) \langle \Phi^{(0)}(\mathbf{y}) \rangle_c d\mathbf{y} \end{aligned} \quad (33)$$

$$\begin{aligned} \sigma_{K\Phi}^2(\mathbf{x}) = - \int_{\Omega} \mathbf{c}_c^{(2)}(\mathbf{x}, \mathbf{y}) \cdot \nabla_{\mathbf{y}} \langle \Phi^{(0)}(\mathbf{y}) \rangle_c d\mathbf{y} \\ - \langle \alpha \rangle \int_{\Omega} c_{c3}^{(2)}(\mathbf{x}, \mathbf{y}) \langle \Phi^{(0)}(\mathbf{y}) \rangle_c d\mathbf{y} \end{aligned} \quad (34)$$

where

$$\tilde{\mathbf{a}}_c^{(2)}(\mathbf{x}, \mathbf{y}) = K_G(\mathbf{x}) K_G(\mathbf{y}) C_Y(\mathbf{y}, \mathbf{x}) \nabla_{\mathbf{x}} \nabla_{\mathbf{y}}^T G(\mathbf{y}, \mathbf{x}) \quad (35)$$

$$\mathbf{a}_c^{(2)}(\mathbf{x}, \mathbf{y}) = K_G(\mathbf{x}) K_G(\mathbf{y}) C_Y(\mathbf{y}, \mathbf{x}) \nabla_{\mathbf{x}} \frac{\partial}{\partial y_3} G(\mathbf{y}, \mathbf{x}) \quad (36)$$

$$\mathbf{c}_c^{(2)}(\mathbf{x}, \mathbf{y}) = K_G(\mathbf{x}) K_G(\mathbf{y}) C_Y(\mathbf{y}, \mathbf{x}) \nabla_{\mathbf{y}} G(\mathbf{y}, \mathbf{x}). \quad (37)$$

Here $C_Y(\mathbf{y}, \mathbf{x}) = \langle Y'(\mathbf{x}) Y'(\mathbf{y}) \rangle_c$ is the conditional covariance of Y' , and the auxiliary function $G(\mathbf{y}, \mathbf{x}) = \langle \mathcal{G}^{(0)}(\mathbf{y}, \mathbf{x}) \rangle_c$ satisfies the deterministic differential equation

$$\begin{aligned} \nabla_{\mathbf{y}} \cdot [K_G(\mathbf{y}) \nabla_{\mathbf{y}} G(\mathbf{y}, \mathbf{x})] - \langle \alpha \rangle K_G(\mathbf{y}) \frac{\partial}{\partial y_3} G(\mathbf{y}, \mathbf{x}) \\ + \delta(\mathbf{y} - \mathbf{x}) = 0 \quad \mathbf{y}, \mathbf{x} \in \Omega \end{aligned} \quad (38)$$

subject to the homogeneous boundary conditions

$$G(\mathbf{y}, \mathbf{x}) = 0 \quad \mathbf{y} \in \Gamma_D \quad (39)$$

$$\nabla_{\mathbf{y}} G(\mathbf{y}, \mathbf{x}) \cdot \mathbf{n} = 0 \quad \mathbf{y} \in \Gamma_N. \quad (40)$$

The first-order approximation $\langle \Phi^{(1)}(\mathbf{x}) \rangle_c \equiv 0$, since it is governed by a homogeneous equation subject to homogeneous boundary conditions.

The zeroth-order approximation of the mean matrix potential, $\langle \Phi(\mathbf{x}) \rangle_c$, satisfies a standard deterministic equation for unsaturated flow in a soil with known properties, driven by mean source and boundary functions. Nonlocality of the mean unsaturated flow equation manifests itself solely at second (and higher) orders which, to our knowledge, have been left out of all previous perturbative stochastic analyses of unsaturated flow.

Appendix A shows that to second order in σ_Y , the conditional autocovariance function $C_\Phi(\mathbf{x}, \mathbf{y}) = \langle \Phi'(\mathbf{x})\Phi'(\mathbf{y}) \rangle_c$ of the Kirchhoff transform Φ is obtained as the solution of the local (partial differential) equation

$$\begin{aligned} \nabla_{\mathbf{x}} \cdot [K_G(\mathbf{x}) \nabla_{\mathbf{x}} C_\Phi^{(2)}(\mathbf{x}, \mathbf{y}) + C_{K\Phi}^{(2)}(\mathbf{x}, \mathbf{y}) \nabla_{\mathbf{x}} \langle \Phi^{(0)}(\mathbf{x}) \rangle_c] \\ + \langle \alpha \rangle \frac{\partial}{\partial x_3} [K_G(\mathbf{x}) C_\Phi^{(2)}(\mathbf{x}, \mathbf{y}) + C_{K\Phi}^{(2)}(\mathbf{x}, \mathbf{y}) \langle \Phi^{(0)}(\mathbf{x}) \rangle_c] = 0 \end{aligned} \quad \mathbf{x} \in \Omega \quad (41)$$

subject to the boundary conditions

$$C_\Phi^{(2)}(\mathbf{x}, \mathbf{y}) = 0 \quad \mathbf{x} \in \Gamma_D \quad (42)$$

$$\begin{aligned} \mathbf{n}(\mathbf{x}) \cdot [K_G(\mathbf{x}) \nabla_{\mathbf{x}} C_\Phi^{(2)}(\mathbf{x}, \mathbf{y}) + C_{K\Phi}^{(2)}(\mathbf{x}, \mathbf{y}) \nabla_{\mathbf{x}} \langle \Phi^{(0)}(\mathbf{x}) \rangle_c] \\ + \langle \alpha \rangle n_3(\mathbf{x}) [K_G(\mathbf{x}) C_\Phi^{(2)}(\mathbf{x}, \mathbf{y}) + C_{K\Phi}^{(2)}(\mathbf{x}, \mathbf{y}) \langle \Phi^{(0)}(\mathbf{x}) \rangle_c] = 0 \end{aligned} \quad \mathbf{x} \in \Gamma_N. \quad (43)$$

A second-order approximation of the conditional cross covariance $C_{K\Phi}(\mathbf{x}, \mathbf{y}) = \langle K'(\mathbf{x})\Phi'(\mathbf{y}) \rangle_c$ is given explicitly by (Appendix A)

$$\begin{aligned} C_{K\Phi}^{(2)}(\mathbf{x}, \mathbf{y}) \\ = -K_G(\mathbf{x}) \int_{\Omega} K_G(\xi) C_Y(\xi, \mathbf{x}) \nabla_{\xi} G(\xi, \mathbf{y}) \cdot \nabla_{\xi} \langle \Phi^{(0)}(\xi) \rangle_c d\xi \\ - \langle \alpha \rangle K_G(\mathbf{x}) \int_{\Omega} K_G(\xi) C_Y(\xi, \mathbf{x}) \frac{\partial G(\xi, \mathbf{y})}{\partial \xi_3} \langle \Phi^{(0)}(\xi) \rangle_c d\xi. \end{aligned} \quad (44)$$

Once the boundary value problems (27)–(29), (30)–(32), and (41)–(43) have been solved, one can continue by developing second-order approximations $\langle \psi^{[2]}(\mathbf{x}) \rangle_c = \langle \psi^{(0)}(\mathbf{x}) \rangle_c + \langle \psi^{(2)}(\mathbf{x}) \rangle_c$ for the mean pressure head and associated second moments, including the variance $[\sigma_\psi^2(\mathbf{x})]^{(2)}$, as described in Appendix B. By virtue of (B4), (B10), and (B11),

$$\langle \psi^{(0)}(\mathbf{x}) \rangle_c = \alpha_G^{-1} \ln [\alpha_G \langle \Phi^{(0)}(\mathbf{x}) \rangle_c] \quad \langle \psi^{(1)}(\mathbf{x}) \rangle_c \equiv 0 \quad (45)$$

$$\langle \psi^{(2)}(\mathbf{x}) \rangle_c = \alpha_G^{-1} \left\{ \langle \Phi^{(2)}(\mathbf{x}) \rangle_c - \frac{1}{2} \frac{[\sigma_\Phi^2(\mathbf{x})]^{(2)}}{\langle \Phi^{(0)}(\mathbf{x}) \rangle_c^2} \right\} \quad (46)$$

$$[\sigma_\psi^2(\mathbf{x})]^{(2)} = \alpha_G^{-2} \frac{[\sigma_\Phi^2(\mathbf{x})]^{(2)}}{\langle \Phi^{(0)}(\mathbf{x}) \rangle_c^2} \quad (47)$$

where $\alpha_G = \exp(\langle \beta \rangle)$ is the geometric mean of α , and $[\sigma_\Phi^2(\mathbf{x})]^{(2)}$ is obtained upon taking the limit of $C_\Phi^{(2)}(\mathbf{x}, \mathbf{y})$ as $\mathbf{y} \rightarrow \mathbf{x}$.

The above systems of deterministic conditional moment

equations involve relatively smooth parameters and dependent variables which are defined on a consistent support scale ω , identical to that of all measurements. As such, these moment equations can be solved either analytically as we do below or, more generally, by standard numerical methods, such as finite elements, on relatively coarse grids without upscaling.

5. One-Dimensional Infiltration

5.1. Analytical Solution

The remainder of this paper is devoted to the development and exploration of an approximate solution for the above moment equations. In particular, we employ perturbation analysis to obtain an analytical solution for one-dimensional infiltration at a constant but random rate Q into a soil column of length L with deterministically prescribed pressure head $\Psi_0 = 0$ at the bottom. Our unconditional solution is nominally valid to second order in σ_Y where $Y(x_3)$ is now a one-dimensional multivariate Gaussian and statistically homogeneous random field with constant mean $\langle Y \rangle$ and an exponential (spatial) autocovariance function

$$C(|x_3 - y_3|) = \sigma_Y^2 \exp\left(-\frac{|x_3 - y_3|}{l_Y}\right) \quad (48)$$

where l_Y is the spatial autocorrelation scale of Y along the vertical coordinate x_3 . Under these conditions, the zeroth-order boundary value problem (27)–(29), and second-order boundary value problems (30)–(32) and (41)–(43), all take the relatively simple form

$$\frac{d^2 \gamma_i(z)}{dz^2} + a \frac{d \gamma_i(z)}{dz} = f_i(z) \quad 0 < z < 1 \quad (49)$$

$$\gamma_i(z) = h_i \quad z = 0 \quad (50)$$

$$\frac{d \gamma_i(z)}{dz} + a \gamma_i(z) = q_i \quad z = 1 \quad (51)$$

where $i = 0, 2, 3$; $z = x_3/L$ is a dimensionless (normalized) vertical coordinate; $a = L \langle \alpha \rangle$ is a dimensionless reciprocal of the macroscopic capillary length; $\gamma_0 = \Phi^{(0)}/L$ and $\gamma_2 = \langle \Phi^{(2)} \rangle/L$ are dimensionless zeroth- and second-order approximations of the mean Kirchhoff potential, respectively; and $\gamma_3 = C_\Phi/L^2$ is a dimensionless covariance of this potential. Corresponding dimensionless source and boundary functions are given, respectively, by

$$f_0(z) \equiv 0$$

$$\begin{aligned} f_2(z) = \frac{d}{dz} \left\{ -\frac{\sigma_Y^2}{2} \frac{d \gamma_0(z)}{dz} - \frac{\sigma_Y^2}{2} a \gamma_0(z) \right. \\ \left. + \frac{r_3^{(2)}(z) - a [\bar{\sigma}_{K\Phi}^2(z)]^{(2)}}{K_G} \right\} \end{aligned} \quad (52)$$

$$f_3(z, \xi) = -\frac{q}{K_G} \frac{d \bar{C}_{K\Phi}^{(2)}(z, \xi)}{dz}$$

where r_3 is the only nonzero component of the residual flux vector $\mathbf{r} = (r_1, r_2, r_3)^T$, and the cross variance $\bar{\sigma}_{K\Phi}^2$ and cross covariance $\bar{C}_{K\Phi}$, given by (C13) and (C14), are both normalized with respect to L ,

$$h_0 = \langle H \rangle/L = a^{-1} \quad h_2 = 0 \quad h_3 = 0 \quad (53)$$

$$q_0 \equiv q = \frac{\langle Q \rangle}{K_G}$$

$$q_2 = -\frac{\sigma_Y^2}{2} \frac{d\gamma_0(1)}{dz} - \frac{\sigma_Y^2}{2} a \gamma_0(1) + \frac{r_3^{(2)}(1) - a[\bar{\sigma}_{K\Phi}^2(1)]^{(2)}}{K_G} \quad (54)$$

$$q_3(\xi) = -\frac{q\bar{C}_{K\Phi}(1, \xi)}{K_G}.$$

Solutions of the boundary value problems (49)–(54), developed in Appendix C, are given explicitly by

$$\gamma_0(z) = \frac{\langle \Phi^{(0)}(z) \rangle}{L} = \frac{q}{a} + \frac{1-q}{a} e^{-az} \quad (55)$$

$$\gamma_2(z) = \frac{\langle \Phi^{(2)}(z) \rangle}{L} = \frac{\sigma_Y^2}{2} \frac{q}{a} (1 - e^{-az}) \quad (56)$$

$$\frac{\gamma_3(z, z)}{\sigma_Y^2 q^2} = \frac{[\sigma_\Phi^2(z)]^{(2)}}{\sigma_Y^2 q^2 L^2}$$

$$= \frac{\lambda}{a(1 - a^2 \lambda^2)} [2a\lambda e^{-(a+1/\lambda)z} - (1 + a\lambda)e^{-2az} + 1 - a\lambda] \quad (57)$$

where $\lambda = l_Y/L$. It is clear from (55) that the zeroth-order approximation of $\langle \Phi(z) \rangle$ does not contain any information about the spatial variability of soil properties; (56) shows that the second-order approximation (in σ_Y) depends only on the variance σ_Y^2 of (natural) log saturated hydraulic conductivity, but not its spatial autocorrelation structure (as expressed by the correlation length λ). To capture dependence on the latter, it would be necessary to consider higher-order terms in the expansion of $\langle \Phi \rangle$. Dependence on λ is restricted in our case to the variance and covariance of Φ .

Substitution of (55)–(57) into (45)–(47) yields expressions for $\langle \psi^{(0)}(z) \rangle$, $\langle \psi^{(2)}(z) \rangle$, and $[\sigma_\psi^2(z)]^{(2)}$.

A very important question which is often overlooked in hydrogeologic perturbation analyses is that of asymptoticity [Dagan and Neuman, 1991]. For the expansion $\langle \Phi \rangle = \langle \Phi^{(0)} \rangle + \langle \Phi^{(2)} \rangle + \dots$ to be asymptotic, it is necessary that $\langle \Phi^{(2)} \rangle \ll \langle \Phi^{(0)} \rangle$. By virtue of (55) and (56) this is equivalent to

$$\frac{\langle \Phi^{(2)}(z) \rangle}{\langle \Phi^{(0)}(z) \rangle} = \frac{\sigma_Y^2}{2} \left\{ 1 + \frac{1}{q[\exp(az) - 1]} \right\}^{-1} \leq \frac{\sigma_Y^2}{2}. \quad (58)$$

Hence our perturbation solution for $\langle \Phi \rangle$ is asymptotic for all $\sigma_Y^2 \leq 2$. This explains why even though our perturbation analysis appears to be nominally restricted to $\sigma_Y^2 \ll 1$, it in fact works quite well (as will soon be seen) for relatively large values of this variance.

5.2. Comparison With Monte Carlo Simulations

We compare below our approximate analytical solution with results of Monte Carlo (MC) simulations generated by solving the corresponding stochastic unsaturated flow equations numerically. The purpose of this comparison is neither to test the appropriateness of our choice of constitutive model, nor to test the validity of our assumptions concerning the spatial statistics of K_s and α ; these have been addressed earlier, and exploring them in greater depth would fall outside the scope of our paper. Instead, we merely want to assess the accuracy of our perturbation solution relative to a numerical Monte Carlo so-

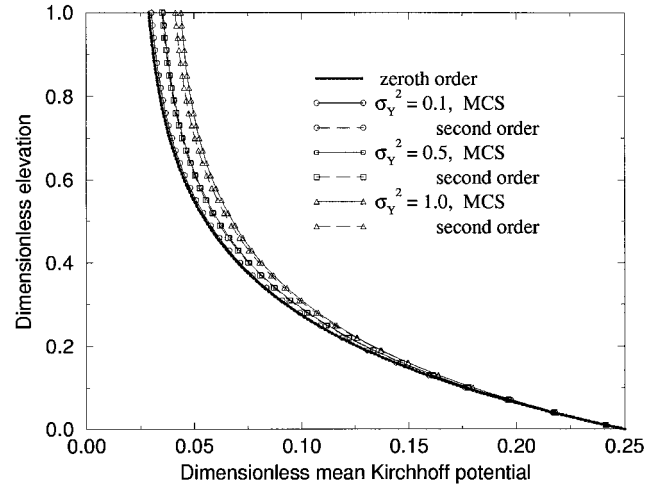


Figure 1. Variation of dimensionless mean Kirchhoff potential with dimensionless elevation for different input variances. MCS denotes Monte Carlo simulation.

lution of the stochastic unsaturated flow equation, from which it derives. For this, we must base both our analytical and numerical solutions on the same constitutive model, parameter statistics, and boundary conditions, as we do below.

We started by investigating the manner in which the dimensionless sample mean Kirchhoff potential $\langle \Phi(z) \rangle/L$, and the normalized sample mean pressure head $\langle \psi(z) \rangle/L$, vary with the number of MC realizations for $a = 4$, $\lambda = 0.1$, $\sigma_Y^2 = 0.5$, and two values of q , 0.1 and 0.3. We found that both sample means reach more or less stable values following about 2000 realizations. We likewise found that the sample variance $\sigma_\Phi^2(z)$ of the Kirchhoff potential and sample variance $\sigma_\psi^2(z)$ of the pressure head, both normalized by $\sigma_Y^2 q^2 L^2$, reach more or less stable values between 4000 and 5000 realizations. Therefore all MC results we present below correspond to 5000 realizations.

Figure 1 compares our zeroth- and second-order (in σ_Y) approximations $\langle \Phi^{[2]} \rangle = \langle \Phi^{(0)} \rangle + \langle \Phi^{(2)} \rangle$ of dimensionless mean Kirchhoff potential with MC results for $a = 4$, $\lambda = 0.1$, $q = 0.1$, and three values of the saturated (natural) log hydraulic conductivity variance σ_Y^2 . Figure 2 shows a similar comparison for dimensionless mean pressure head. Both figures clearly demonstrate the superiority of the second-order over the zeroth-order perturbation solution. Though the perturbation solution is nominally valid only for $\sigma_Y^2 \ll 1$, we see that the second-order approximation compares well with MC results even for $\sigma_Y^2 = 1$, though its quality improves as σ_Y^2 diminishes. An increase in σ_Y^2 is seen to be accompanied by an increase in mean Kirchhoff potential and pressure head. The effect of σ_Y^2 on both quantities increases monotonically with vertical distance from the prescribed potential boundary at the bottom, toward the prescribed flux boundary at the top.

Figure 3 compares our second-order approximation of the dimensionless variance σ_Φ^2 of Kirchhoff potential with MC results for the same parameters as those in Figures 1 and 2. The comparison is acceptable for the very small input variance $\sigma_Y^2 = 0.1$ but poor for $\sigma_Y^2 \geq 0.5$, suggesting that it may be necessary to develop a fourth-order approximation (second order in σ_Y^2) to obtain improved analytical predictions of σ_Φ^2 . The comparison is, however, much better for the dimensionless variance σ_ψ^2 of pressure head in Figure 4. We attribute this

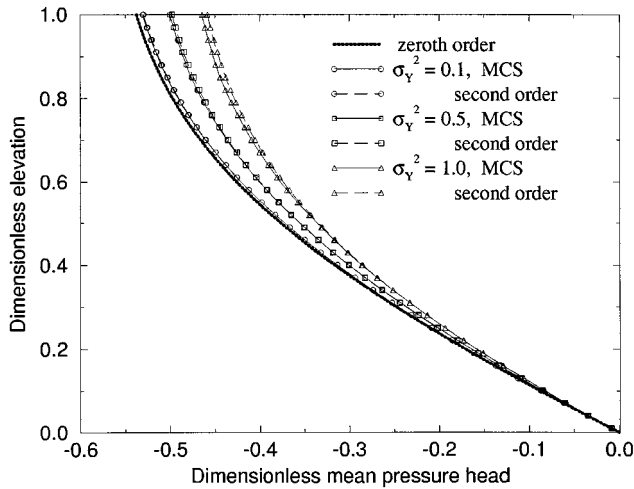


Figure 2. Variation of dimensionless mean pressure head with dimensionless elevation for different input variances.

to the fact that Φ is exponential in ψ and present from now on only results corresponding to moments of pressure head. An increase in σ_Y^2 is seen to cause a large relative increase in the variance of the Kirchhoff potential and a much smaller relative increase in the variance of the pressure head. The variance of both quantities is zero at the bottom prescribed potential boundary and increases monotonically toward the prescribed flux boundary at the top.

Figure 5 shows dimensionless mean pressure head for $a = 4$, $\lambda = 0.1$, $\sigma_Y^2 = 0.5$ and several values of q ; Figure 6 depicts the corresponding dimensionless variance. The agreement between second-order analytical and MC solutions is acceptable in both cases; we found (but do not show) that it is nearly perfect when $\sigma_Y^2 = 0.1$. This agreement generally decreases as q increases. The agreement between zeroth-order and MC results is, for the most part, less satisfactory; the same holds true to a lesser extent for $\sigma_Y^2 = 0.1$ (not shown). Both dimensionless pressure head moments are sensitive to dimensionless flux: Whereas the mean increases with q , the variance decreases with the same quantity. The effect of a on these two

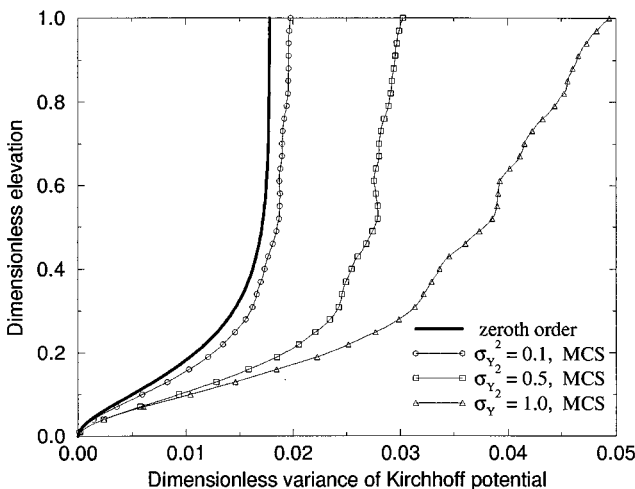


Figure 3. Variation of dimensionless variance of Kirchhoff potentials with dimensionless elevation for different input variances.

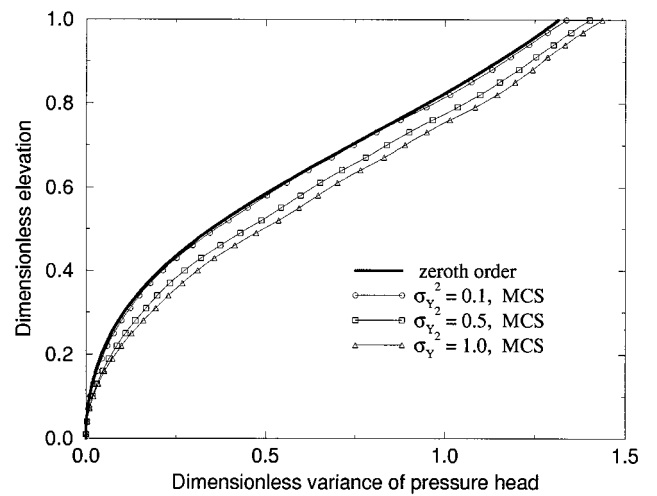


Figure 4. Variation of dimensionless variance of pressure heads with dimensionless elevation for different input variances.

dimensionless pressure head moments is illustrated in Figures 7 and 8, respectively, for $\sigma_Y^2 = 0.5$, $\lambda = 0.1$, and $q = 0.1$. Whereas both moments are sensitive to the dimensionless mean reciprocal capillary length scale, the dimensionless mean pressure head increases with a while the dimensionless variance first increases and then decreases. Figures 9 and 10 help elucidate the effect that λ has on the dimensionless moments of pressure head. Whereas the normalized mean pressure head decreases as λ increases, the corresponding variance increases at a relatively fast rate. The agreement between second-order and MC results is excellent in the case of normalized mean pressure head and satisfactory in the case of its normalized variance; it becomes near perfect when $\sigma_Y^2 = 0.1$ (not shown).

Figures 11–16 depict results analogous to those in Figures 5–10 but for the nominal upper limit of our perturbation expansion, $\sigma_Y^2 = 1$. As the accuracy of the zeroth-order solution decreases with an increase in σ_Y^2 , the value of our second-order solution becomes more evident. The accuracy of the latter is very good for some values of q , a , and λ , but not so good for others. The overall behavior of the solution is preserved even

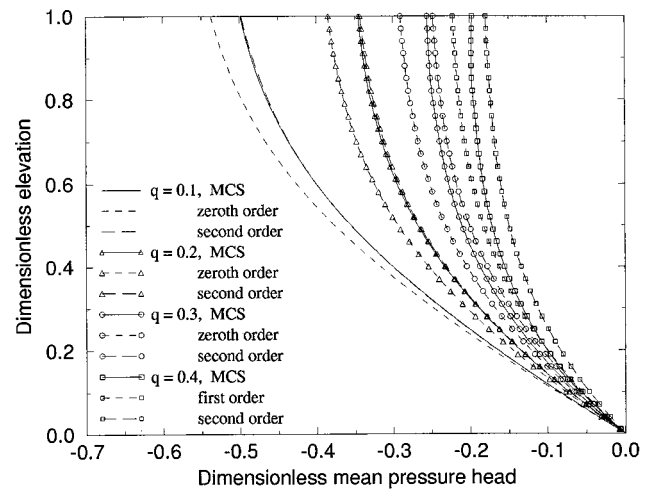


Figure 5. Variation of dimensionless mean pressure head with dimensionless elevation for different values of q when $\sigma_Y^2 = 0.5$.

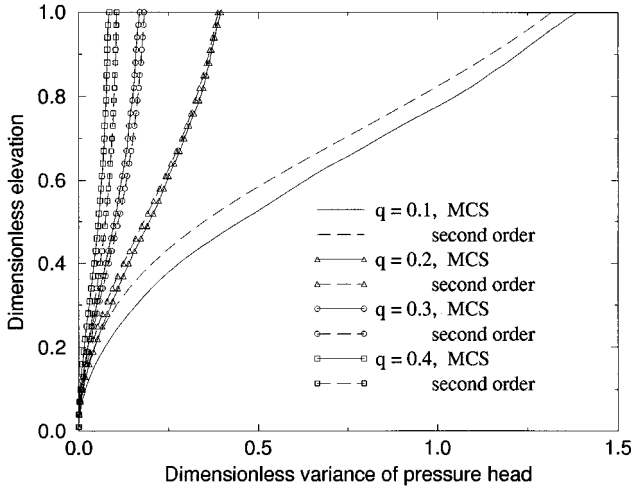


Figure 6. Variation of dimensionless variance of pressure heads with dimensionless elevation for different values of q when $\sigma_\gamma^2 = 0.5$.

as the accuracy of the analytical solution generally deteriorates with an increase in λ .

We end by noting that our solution was obtained without explicit use of the Taylor expansion

$$\begin{aligned} \langle K(\psi) \rangle &= \langle K(\langle \psi \rangle + \psi') \rangle \\ &= \langle K(\langle \psi \rangle) \rangle + \frac{1}{2} \frac{d^2 \langle K(s) \rangle}{ds^2} \bigg|_{s=\langle \psi \rangle} \sigma_\psi^2 + O(\langle \psi'^3 \rangle) \end{aligned} \quad (59)$$

which we can therefore use to explore the validity of the common approximation $\langle K_r(\psi) \rangle \approx \langle K_r(\langle \psi \rangle) \rangle$. It follows from (5) that

$$\langle K_r(\psi) \rangle \approx e^{\alpha_G \langle \psi^{(2)} \rangle} \left\{ 1 + \frac{\alpha_G^2}{2} [\sigma_\psi^2]^{(2)} + \dots \right\} \quad (60)$$

Hence the approximation $\langle K_r(\psi) \rangle \approx \langle K_r(\langle \psi \rangle) \rangle$ is valid when $\alpha_G^2 [\sigma_\psi^2]^{(2)} / 2 \ll 1$; on the other hand, the Taylor expansion converges provided only that $\alpha_G^2 [\sigma_\psi^2]^{(2)} / 2 < 1$.

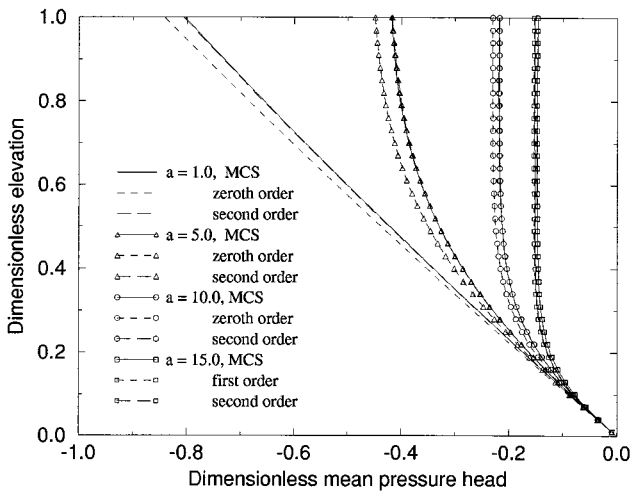


Figure 7. Variation of dimensionless mean pressure head with dimensionless elevation for different values of a when $\sigma_\gamma^2 = 0.5$.

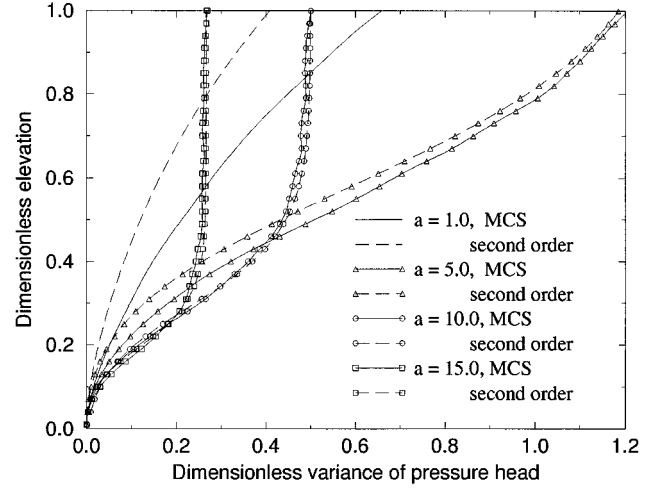


Figure 8. Variation of dimensionless variance of pressure heads with dimensionless elevation for different values of a when $\sigma_\gamma^2 = 0.5$.

6. Conclusions

1. We described a deterministic alternative to (conditional) Monte Carlo simulation, which allows predicting steady state unsaturated flow under uncertainty, and assessed the latter by means of conditional second moments, without having to generate random fields or variables, without upscaling, and without linearizing the constitutive characteristics of the soil. Such prediction is possible by means of first ensemble moments of system states and fluxes, conditioned on measured values of soil properties, when the latter scale in a linearly separable fashion. In the particular case where the scaling parameter of pressure head is a random variable independent of location, the steady state unsaturated flow equation can be linearized by means of the Kirchhoff transformation for gravity-free flow. Linearization is also possible in the presence of gravity when hydraulic conductivity varies exponentially with pressure head. We developed exact nonlocal (integrodifferential) conditional moment equations for the latter situation

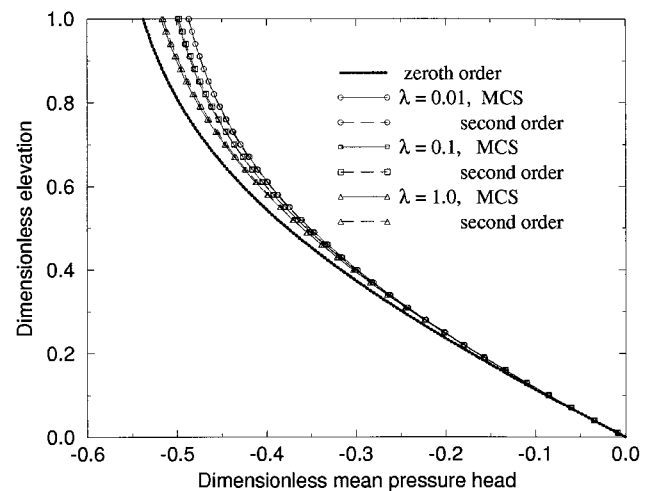


Figure 9. Variation of dimensionless mean pressure head with dimensionless elevation for different values of λ when $\sigma_\gamma^2 = 0.5$.

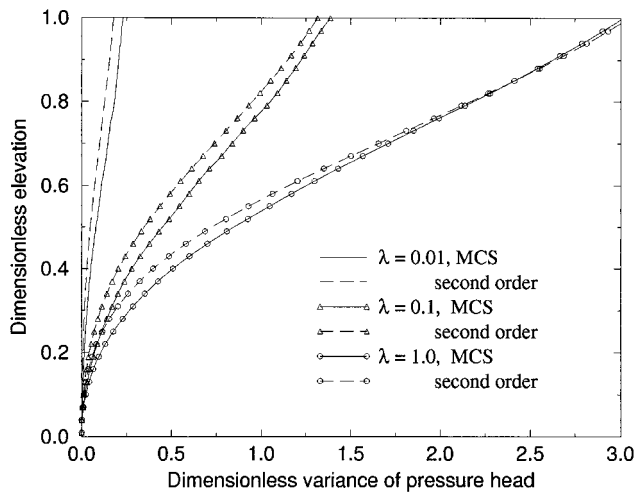


Figure 10. Variation of dimensionless variance of pressure heads with dimensionless elevation for different values of λ when $\sigma_Y^2 = 0.5$.

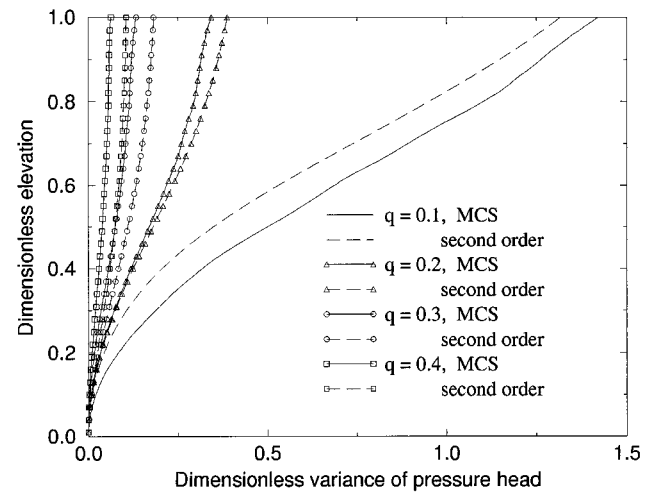


Figure 12. Variation of dimensionless variance of pressure heads with dimensionless elevation for different values of q when $\sigma_Y^2 = 1$.

which contain parameters that are conditional on data and therefore nonunique. The conditional mean solution constitutes an optimum unbiased predictor of the otherwise unknown state of the system, and conditional second moments provide a measure of the corresponding prediction uncertainty.

2. The derivation of moment equations for soils whose properties do not scale in the above manner requires linearizing the corresponding constitutive relations. This may lead to major inaccuracies when these relations are highly nonlinear, as is often the case in nature. Virtually all previously published moment analyses of unsaturated flow, whether analytical or numerical, have found it necessary to rely on perturbative approximations of soil constitutive relations. We have shown how one can preserve the nonlinear nature of *Gardner's* [1958] exponential relationship between hydraulic conductivity and pressure head in a stochastic moment analysis of steady state flow under gravity by using the Kirchhoff transformation. This requires that we treat the exponent α in this relationship as a

random constant rather than a spatially varying random field. Though this is an important limitation, a survey of the literature concerning the spatial variability of α has convinced us that this is a relatively small price to pay for the advantage of preserving constitutive nonlinearity.

3. We showed rigorously that the concept of effective hydraulic conductivity does not generally apply to statistically averaged unsaturated flow equations except when they are unconditional and flow is driven solely by gravity.

4. All conditional parameters and moments in our equations are defined on the same consistent measurement (support) scale ω as the data. This obviates the need for upscaling, though one can easily integrate the conditional mean solution in space-time if one so desires.

5. Though our conditional moment equations are mathematically exact, they nevertheless require a closure approximation to be workable. The approximation we use is based on perturbation analysis, which leads to recursive equations that can be solved either analytically, as we have done here, or by

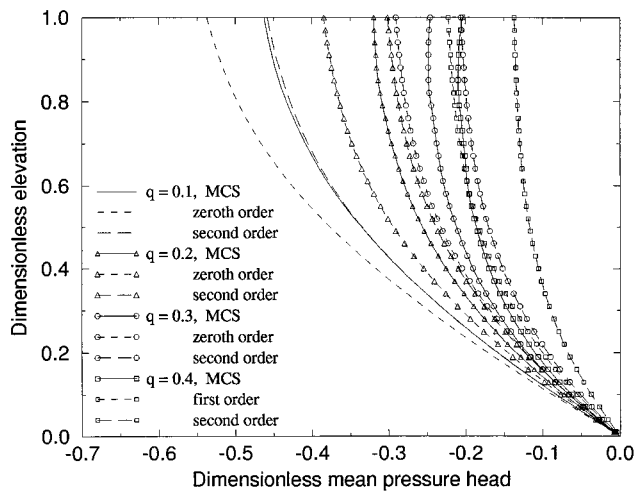


Figure 11. Variation of dimensionless mean pressure head with dimensionless elevation for different values of q when $\sigma_Y^2 = 1$.

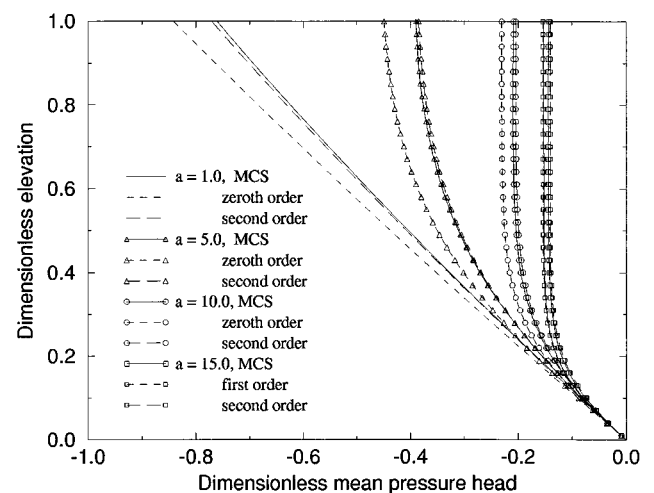


Figure 13. Variation of dimensionless mean pressure head with dimensionless elevation for different values of a when $\sigma_Y^2 = 1$.

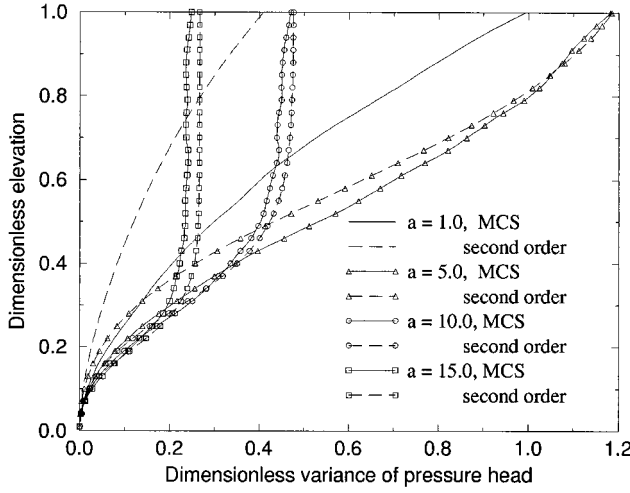


Figure 14. Variation of dimensionless variance of pressure heads with dimensionless elevation for different values of a when $\sigma_Y^2 = 1$.

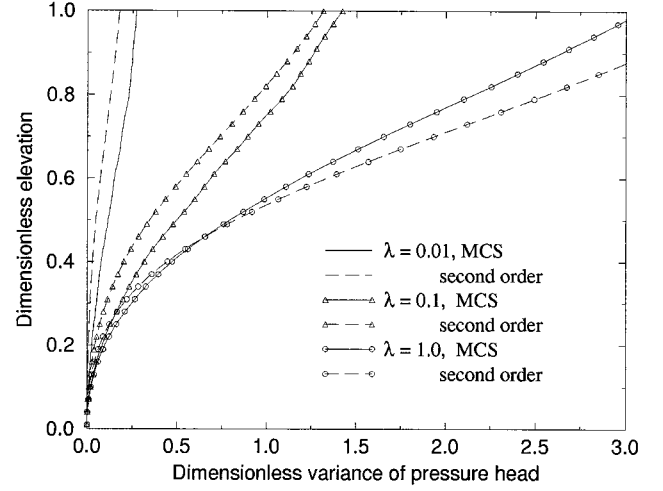


Figure 16. Variation of dimensionless variance of pressure heads with dimensionless elevation for different values of λ when $\sigma_Y^2 = 1$.

standard numerical methods such as the recent finite element solution of the steady state saturated flow problem by *Guadagnini and Neuman* [1997, 1998]. Perturbative solutions are nominally limited to soils that are either mildly heterogeneous or strongly heterogeneous but with well-conditioned estimates of hydraulic properties. We nevertheless expect them to work quite well even for strongly heterogeneous soils without extensive conditioning; our optimism is based on the quality of unconditional analytical results in this paper, on our formal analysis of asymptoticity, and on the experience of Guadagnini and Neuman.

6. All conditional parameters and moments in our equations are smooth relative to their random counterpart and can therefore be resolved, in principle, on a numerical grid which is coarser than that typically required for the Monte Carlo simulation of random fields.

7. We developed analytical solutions for the Kirchhoff potential, pressure head, and their variances under vertical infil-

tration, without conditioning, to second order in the (input) standard deviation of natural log saturated hydraulic conductivity (first order in its variance). We then compared these with Monte Carlo results obtained by solving the stochastic Richards equation numerically. Our second-order approximations are generally far superior to zeroth-order approximations, and the variance of pressure heads compares much better with Monte Carlo values than does the variance of Kirchhoff potentials. Both the analytical pressure head and its variances compare well with Monte Carlo results for input variances at least as large as 1. This accords well with theoretical analysis which shows that our analytical solution remains asymptotic for input variances as large as 2.

Appendix A

Subtracting (14) and (15) from (8) gives the following equation for the perturbations $\Phi'(\mathbf{x})$,

$$\begin{aligned} \nabla \cdot [K_s(\mathbf{x}) \nabla \Phi'(\mathbf{x}) + K'_s(\mathbf{x}) \nabla \langle \Phi(\mathbf{x}) \rangle_c + \mathbf{r}_c(\mathbf{x})] \\ + \frac{\partial}{\partial x_3} [\alpha K_s(\mathbf{x}) \Phi'(\mathbf{x}) + \alpha' K_s(\mathbf{x}) \langle \Phi(\mathbf{x}) \rangle_c + \langle \alpha \rangle K'_s(\mathbf{x}) \\ \cdot \langle \Phi(\mathbf{x}) \rangle_c - \langle \alpha \rangle \sigma_{K\Phi}^2(\mathbf{x}) - \langle K_s(\mathbf{x}) \rangle_c \sigma_{\alpha\Phi}^2(\mathbf{x}) \\ - \langle \alpha' K'_s(\mathbf{x}) \Phi'(\mathbf{x}) \rangle_c] + f'(\mathbf{x}) = 0 \quad \mathbf{x} \in \Omega. \end{aligned} \quad (\text{A1})$$

A similar procedure yields the boundary conditions

$$\Phi'(\mathbf{x}) = H'(\mathbf{x}) \quad \mathbf{x} \in \Gamma_D \quad (\text{A2})$$

$$\begin{aligned} \mathbf{n}(\mathbf{x}) \cdot [K_s(\mathbf{x}) \nabla \Phi'(\mathbf{x}) + K'_s(\mathbf{x}) \nabla \langle \Phi(\mathbf{x}) \rangle_c + \mathbf{r}_c(\mathbf{x})] + n_3(\mathbf{x}) \\ \cdot [\alpha K_s(\mathbf{x}) \Phi'(\mathbf{x}) + \alpha' K_s(\mathbf{x}) \langle \Phi(\mathbf{x}) \rangle_c + \langle \alpha \rangle K'_s(\mathbf{x}) \langle \Phi(\mathbf{x}) \rangle_c \\ - \langle \alpha \rangle \sigma_{K\Phi}^2(\mathbf{x}) - \langle K_s(\mathbf{x}) \rangle_c \sigma_{\alpha\Phi}^2(\mathbf{x}) - \langle \alpha' K'_s(\mathbf{x}) \Phi'(\mathbf{x}) \rangle_c] \\ = Q'(\mathbf{x}) \quad \mathbf{x} \in \Gamma_N. \end{aligned} \quad (\text{A3})$$

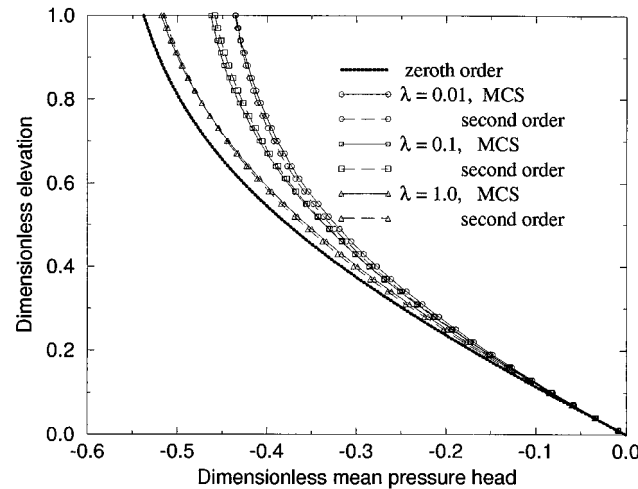


Figure 15. Variation of dimensionless mean pressure head with dimensionless elevation for different values of λ when $\sigma_Y^2 = 1$.

Expressing (A1) in terms of \mathbf{y} , multiplying by $\mathcal{G}(\mathbf{y}, \mathbf{x})$, and integrating over Ω gives

$$\begin{aligned}
& \int_{\Omega} \left\{ \nabla_{\mathbf{y}} \cdot [K_s(\mathbf{y}) \nabla_{\mathbf{y}} \Phi'(\mathbf{y})] + \alpha \frac{\partial}{\partial y_3} [K_s(\mathbf{y}) \Phi'(\mathbf{y})] \right\} \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} \\
& + \int_{\Omega} \frac{\partial}{\partial y_3} [\alpha' K_s(\mathbf{y}) \langle \Phi(\mathbf{y}) \rangle_c + \langle \alpha \rangle K_s'(\mathbf{y}) \langle \Phi(\mathbf{y}) \rangle_c \\
& - \langle \alpha \rangle \sigma_{K\Phi}^2(\mathbf{y}) - \langle K_s(\mathbf{y}) \rangle_c \sigma_{\alpha\Phi}^2(\mathbf{y}) \\
& - \langle \alpha' K_s'(\mathbf{y}) \Phi'(\mathbf{y}) \rangle_c] \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} \\
& + \int_{\Omega} \nabla_{\mathbf{y}} \cdot [K_s'(\mathbf{y}) \nabla_{\mathbf{y}} \langle \Phi(\mathbf{y}) \rangle_c + \mathbf{r}_c(\mathbf{y})] \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} \\
& + \int_{\Omega} f'(\mathbf{y}) \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} = 0. \tag{A4}
\end{aligned}$$

Applying Green's formula to the first integral, integrating the second integral by parts, applying Green's identity to the remaining divergence integral, and recalling the definition of $\mathcal{G}(\mathbf{y}, \mathbf{x})$ yields, by virtue of (A2) and (A3),

$$\begin{aligned}
\Phi'(\mathbf{x}) &= - \int_{\Omega} [K_s'(\mathbf{y}) \nabla_{\mathbf{y}} \langle \Phi(\mathbf{y}) \rangle_c + \mathbf{r}_c(\mathbf{y})] \cdot \nabla_{\mathbf{y}} \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} \\
& - \int_{\Omega} [\alpha' K_s(\mathbf{y}) \langle \Phi(\mathbf{y}) \rangle_c + \langle \alpha \rangle K_s'(\mathbf{y}) \langle \Phi(\mathbf{y}) \rangle_c - \langle \alpha \rangle \sigma_{K\Phi}^2(\mathbf{y}) \\
& - \langle K_s(\mathbf{y}) \rangle_c \sigma_{\alpha\Phi}^2(\mathbf{y}) - \langle \alpha' K_s'(\mathbf{y}) \Phi'(\mathbf{y}) \rangle_c] \frac{\partial}{\partial y_3} \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} \\
& + \int_{\Omega} f'(\mathbf{y}) \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} - \int_{\Gamma_D} H'(\mathbf{y}) K_s(\mathbf{y}) \frac{\partial}{\partial n} \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y} \\
& + \int_{\Gamma_N} Q'(\mathbf{y}) \mathcal{G}(\mathbf{y}, \mathbf{x}) d\mathbf{y}. \tag{A5}
\end{aligned}$$

Operating on (A5) with the stochastic differential operator $K_s'(\mathbf{x}) \nabla_{\mathbf{x}}$, taking conditional ensemble mean, and accounting for statistical independence of the randomly prescribed source and boundary functions leads directly to (18), (20), and (21). By the same token, multiplying (A5) by $K_s'(\mathbf{x})$ and taking conditional ensemble mean leads to (19) and (22); multiplying (A5) by α' and taking conditional ensemble mean leads to an analogous equation for $\sigma_{\alpha\Phi}^2(\mathbf{x})$.

A boundary value problem for the conditional covariance function $C_{\Phi}(\mathbf{x}, \mathbf{y}) = \langle \Phi'(\mathbf{x}) \Phi'(\mathbf{y}) \rangle_c$ can be obtained upon multiplying (A1)–(A3) by $\Phi'(\mathbf{y})$ and taking conditional ensemble mean,

$$\begin{aligned}
& \nabla_{\mathbf{x}} \cdot [\langle K_s(\mathbf{x}) \rangle_c \nabla_{\mathbf{x}} C_{\Phi}(\mathbf{x}, \mathbf{y}) + \langle K_s'(\mathbf{x}) \nabla_{\mathbf{x}} \Phi'(\mathbf{y}) \Phi'(\mathbf{x}) \rangle_c \\
& + C_{K\Phi}(\mathbf{x}, \mathbf{y}) \nabla_{\mathbf{x}} \langle \Phi(\mathbf{x}) \rangle_c] + \langle \alpha \rangle \frac{\partial}{\partial x_3} [\langle K_s(\mathbf{x}) \rangle_c C_{\Phi}(\mathbf{x}, \mathbf{y}) \\
& + \langle K_s'(\mathbf{x}) \Phi'(\mathbf{y}) \Phi'(\mathbf{x}) \rangle_c + C_{K\Phi}(\mathbf{x}, \mathbf{y}) \langle \Phi(\mathbf{x}) \rangle_c] = 0 \\
& \mathbf{x}, \mathbf{y} \in \Omega \tag{A6}
\end{aligned}$$

subject to

$$C_{\Phi}(\mathbf{x}, \mathbf{y}) = 0 \quad \mathbf{x} \in \Gamma_D \tag{A7}$$

$$\begin{aligned}
& \mathbf{n}(\mathbf{x}) \cdot [\langle K_s(\mathbf{x}) \rangle_c \nabla_{\mathbf{x}} C_{\Phi}(\mathbf{x}, \mathbf{y}) + \langle K_s'(\mathbf{x}) \nabla_{\mathbf{x}} \Phi'(\mathbf{y}) \Phi'(\mathbf{x}) \rangle_c \\
& + C_{K\Phi}(\mathbf{x}, \mathbf{y}) \nabla_{\mathbf{x}} \langle \Phi(\mathbf{x}) \rangle_c] + \langle \alpha \rangle n_3(\mathbf{x}) [\langle K_s(\mathbf{x}) \rangle_c C_{\Phi}(\mathbf{x}, \mathbf{y}) \\
& + \langle K_s'(\mathbf{x}) \Phi'(\mathbf{y}) \Phi'(\mathbf{x}) \rangle_c + C_{K\Phi}(\mathbf{x}, \mathbf{y}) \langle \Phi(\mathbf{x}) \rangle_c] = 0 \\
& \mathbf{x} \in \Gamma_N. \tag{A8}
\end{aligned}$$

The cross-covariance function $C_{K\Phi}(\mathbf{x}, \mathbf{y}) = \langle K'(\mathbf{x}) \Phi'(\mathbf{y}) \rangle_c$ is obtained upon expressing (A5) in terms of \mathbf{y} , multiplying by $K_s'(\mathbf{x})$, and taking conditional ensemble mean,

$$\begin{aligned}
C_{K\Phi}(\mathbf{x}, \mathbf{y}) &= - \int_{\Omega} \langle K_s'(\mathbf{x}) K_s'(\xi) \nabla_{\xi} \mathcal{G}(\xi, \mathbf{y}) \rangle_c \cdot \nabla_{\xi} \langle \Phi(\xi) \rangle_c d\xi \\
& - \int_{\Omega} \langle K_s'(\mathbf{x}) K_s'(\xi) \nabla_{\xi} \mathcal{G}(\xi, \mathbf{y}) \rangle_c \cdot \mathbf{r}_c(\xi) d\xi \\
& - \langle \alpha \rangle \int_{\Omega} \left\langle K_s'(\mathbf{x}) K_s'(\xi) \frac{\partial}{\partial \xi_3} \mathcal{G}(\xi, \mathbf{y}) \right\rangle_c \langle \Phi(\xi) \rangle_c d\xi \\
& + \langle \alpha \rangle \int_{\Omega} \left\langle K_s'(\mathbf{x}) \frac{\partial}{\partial \xi_3} \mathcal{G}(\xi, \mathbf{y}) \right\rangle_c \sigma_{K\Phi}^2(\xi) d\xi. \tag{A9}
\end{aligned}$$

Appendix B

The following identities are used in our perturbation analysis:

$$\langle K_s \rangle_c = \langle e^Y \rangle_c = K_G \langle e^{Y'} \rangle_c = K_G \left[1 + \frac{\sigma_Y^2}{2} + O(\langle Y'^3 \rangle_c) \right] \tag{B1}$$

$$\begin{aligned}
K_s' &= K_s - \langle K_s \rangle_c = K_G [e^{Y'} - \langle e^{Y'} \rangle_c] \\
&= K_G \left[Y' + \frac{Y'^2}{2} - \frac{\sigma_Y^2}{2} + O(Y'^3) \right] \tag{B2}
\end{aligned}$$

where $K_G = e^{\langle Y \rangle_c}$ is the geometric mean of the saturated hydraulic conductivity K_s and $\sigma_Y^2 = \langle Y' Y' \rangle_c$ is the variance of the natural log saturated hydraulic conductivity Y .

Taking conditional ensemble mean of (7) yields

$$\langle \alpha \rangle \langle \Phi(\mathbf{x}) \rangle_c = \langle e^{\alpha \langle \psi(\mathbf{x}) \rangle_c} (1 + \alpha \psi'(\mathbf{x}) + \frac{1}{2} \alpha^2 \psi'^2(\mathbf{x}) + \dots) \rangle_c. \tag{B3}$$

Collecting terms of the same powers of σ_Y gives

$$\langle e^{\alpha \langle \psi^{(0)}(\mathbf{x}) \rangle_c} \rangle = \langle \alpha \rangle \langle \Phi^{(0)}(\mathbf{x}) \rangle_c \quad \langle \psi^{(1)}(\mathbf{x}) \rangle_c \equiv 0 \tag{B4}$$

$$\begin{aligned}
& \langle \alpha e^{\alpha \langle \psi^{(0)}(\mathbf{x}) \rangle_c} \rangle \langle \psi^{(2)}(\mathbf{x}) \rangle_c + \frac{1}{2} \langle \alpha^2 e^{\alpha \langle \psi^{(0)}(\mathbf{x}) \rangle_c} \rangle [\sigma_{\psi}^2(\mathbf{x})]^{(2)} \\
& = \langle \alpha \rangle \langle \Phi^{(2)}(\mathbf{x}) \rangle_c. \tag{B5}
\end{aligned}$$

Since (B5) contains two unknowns, $\langle \psi^{(2)}(\mathbf{x}) \rangle_c$ and $[\sigma_{\psi}^2(\mathbf{x})]^{(2)}$, there is a need for an additional equation. From (7) it follows that $\alpha^2 \Phi^2 = \exp(2\alpha\psi)$. Taking conditional ensemble mean yields

$$\langle \alpha^2 \rangle \langle \Phi^2(\mathbf{x}) \rangle_c = \langle e^{2\alpha \langle \psi(\mathbf{x}) \rangle_c} (1 + 2\alpha \psi'(\mathbf{x}) + 2\alpha^2 \psi'^2(\mathbf{x}) + \dots) \rangle_c. \tag{B6}$$

Collecting terms of order σ_Y^2 gives

$$\begin{aligned} & \langle \alpha e^{2\alpha\langle\psi^{(0)}(\mathbf{x})\rangle_c} \rangle \langle \psi^{(2)}(\mathbf{x}) \rangle_c + \langle \alpha^2 e^{2\alpha\langle\psi^{(0)}(\mathbf{x})\rangle_c} [\sigma_\psi^2(\mathbf{x})]^{(2)} \rangle \\ &= \langle \alpha^2 \rangle \langle \Phi^{(0)}(\mathbf{x}) \rangle_c \langle \Phi^{(2)}(\mathbf{x}) \rangle_c + \frac{\langle \alpha^2 \rangle}{2} [\sigma_\Phi^2(\mathbf{x})]^{(2)}. \end{aligned} \quad (\text{B7})$$

It likewise follows from (7) that

$$\langle \alpha e^{\alpha\langle\psi^{(0)}(\mathbf{x})\rangle_c} \rangle = \langle \alpha^2 \rangle \langle \Phi^{(0)}(\mathbf{x}) \rangle_c \quad (\text{B8})$$

$$\langle \alpha^2 e^{\alpha\langle\psi^{(0)}(\mathbf{x})\rangle_c} \rangle = \langle \alpha^3 \rangle \langle \Phi^{(0)}(\mathbf{x}) \rangle_c$$

$$\langle \alpha e^{2\alpha\langle\psi^{(0)}(\mathbf{x})\rangle_c} \rangle = \langle \alpha^3 \rangle \langle \Phi^{(0)}(\mathbf{x}) \rangle_c \quad (\text{B9})$$

$$\langle \alpha^2 e^{2\alpha\langle\psi^{(0)}(\mathbf{x})\rangle_c} \rangle = \langle \alpha^4 \rangle \langle \Phi^{(0)}(\mathbf{x}) \rangle_c.$$

Substituting (B8) into (B5), and (B9) into (B7), yields a system of two linear algebraic equations,

$$\langle \psi^{(2)}(\mathbf{x}) \rangle_c + \frac{1}{2} \frac{\langle \alpha^3 \rangle}{\langle \alpha^2 \rangle} [\sigma_\psi^2(\mathbf{x})]^{(2)} = \frac{\langle \alpha \rangle}{\langle \alpha^2 \rangle} \frac{\langle \Phi^{(2)}(\mathbf{x}) \rangle_c}{\langle \Phi^{(0)}(\mathbf{x}) \rangle_c} \quad (\text{B10})$$

$$\begin{aligned} & \langle \psi^{(2)}(\mathbf{x}) \rangle_c + \frac{\langle \alpha^4 \rangle}{\langle \alpha^3 \rangle} [\sigma_\psi^2(\mathbf{x})]^{(2)} = \frac{\langle \alpha^2 \rangle}{\langle \alpha^3 \rangle} \frac{\langle \Phi^{(2)}(\mathbf{x}) \rangle_c}{\langle \Phi^{(0)}(\mathbf{x}) \rangle_c} \\ & + \frac{1}{2} \frac{\langle \alpha^2 \rangle}{\langle \alpha^3 \rangle} \frac{[\sigma_\Phi^2(\mathbf{x})]^{(2)}}{\langle \Phi^{(0)}(\mathbf{x}) \rangle_c^2}. \end{aligned} \quad (\text{B11})$$

Appendix C

The dimensionless auxiliary function $G_K(\zeta, z)$ is the solution of the one-dimensional version of (38) written in dimensionless coordinates $z = y_3/L$ and $\zeta = x_3/L$,

$$\frac{d^2 G_K(z, \zeta)}{dz^2} - a \frac{dG_K(z, \zeta)}{dz} + \delta(z - \zeta) = 0 \quad (\text{C1})$$

$$0 < z, \zeta < 1$$

subject to one-dimensional version of the boundary conditions (39) and (40),

$$G_K(z, \zeta) = 0 \quad z = 0 \quad (\text{C2})$$

$$\frac{dG_K(z, \zeta)}{dz} \quad z = 1. \quad (\text{C3})$$

By direct substitution into (C1)–(C3), one can easily verify that such $G_K(z, \zeta)$ is then given by

$$G_K(z, \zeta) = \frac{1}{a} e^{-a\zeta} (e^{az} - 1) \quad 0 \leq z \leq \zeta \quad (\text{C4})$$

$$G_K(z, \zeta) = \frac{1}{a} (1 - e^{-a\zeta}) \quad \zeta \leq z \leq 1.$$

Note that since the differential operator in (38) is not self-adjoint, the auxiliary function $G_K(z, \zeta)$ is not symmetric with respect to its arguments.

Introducing a new dependent variable $\phi_i(z) = \gamma_i \exp(az/2)$ transforms the boundary value problem (49)–(51) into its self-adjoint form

$$\frac{d^2 \phi_i(z)}{dz^2} - b^2 \phi_i(z) = f_i(z) e^{bz} \quad 0 < z < 1 \quad (\text{C5})$$

$$\phi_i(z) = h_i \quad z = 0 \quad (\text{C6})$$

$$\frac{d\phi_i(z)}{dz} + b\phi_i(z) = q_i e^{bz} \quad z = 1 \quad (\text{C7})$$

where $b = a/2$. A symmetric Green's function $g(z, \zeta)$ associated with (C5)–(C7) is given by

$$\begin{aligned} g(z, \zeta) &= -\frac{1}{b} e^{-b\zeta} \sinh(bz) \quad 0 \leq z \leq \zeta \\ g(z, \zeta) &= -\frac{1}{b} e^{-bz} \sinh(b\zeta) \quad \zeta \leq z \leq 1, \end{aligned} \quad (\text{C8})$$

so that the general solution of (C5)–(C7) can be expressed as

$$\begin{aligned} \phi_i(z) &= -\frac{e^{-bz}}{b} \int_0^z f_i(\zeta) e^{b\zeta} \sinh(b\zeta) d\zeta \\ &- \sinh(bz) \int_z^1 f_i(\zeta) d\zeta + \frac{q_i}{b} \sinh(bz) + h_i e^{-bz}. \end{aligned} \quad (\text{C9})$$

Substituting f_0 , h_0 , and q_0 from (52)–(54) into (C9) leads directly to (55).

For one-dimensional infiltration, (33)–(37) and (44) reduce to

$$\begin{aligned} \frac{r_3^{(2)}(x_3)}{K_G} &= \int_0^L \left[\frac{\partial \langle \Phi^{(0)}(y_3) \rangle}{\partial y_3} + \langle \alpha \rangle \langle \Phi^{(0)}(y_3) \rangle \right] \\ &\cdot C_Y(|x_3 - y_3|) \frac{\partial^2 G_K(y_3, x_3)}{\partial x_3 \partial y_3} dy_3 \end{aligned} \quad (\text{C10})$$

$$\begin{aligned} \frac{\sigma_{K\Phi}^{(2)}(x_3)}{K_G} &= -\int_0^L \left[\frac{\partial \langle \Phi^{(0)}(y_3) \rangle}{\partial y_3} + \langle \alpha \rangle \langle \Phi^{(0)}(y_3) \rangle \right] \\ &\cdot C_Y(|x_3 - y_3|) \frac{\partial G_K(y_3, x_3)}{\partial y_3} dy_3 \end{aligned} \quad (\text{C11})$$

$$\begin{aligned} \frac{C_{K\Phi}^{(2)}(x_3, y_3)}{K_G} &= -\int_0^L \left[\frac{\partial \langle \Phi^{(0)}(\xi_3) \rangle}{\partial \xi_3} + \langle \alpha \rangle \langle \Phi^{(0)}(\xi_3) \rangle \right] \\ &\cdot C_Y(|x_3 - \xi_3|) \frac{\partial G_K(\xi_3, y_3)}{\partial \xi_3} d\xi_3. \end{aligned} \quad (\text{C12})$$

Switching to the dimensionless variable $\zeta = x_3/L$, substituting C_Y from (48) and G_K from (C4), and evaluating the integral leads to

$$\begin{aligned} \frac{r_3^{(2)}(\zeta)}{\sigma_Y^2 K_G q} &= \frac{1}{1 + a\lambda} [1 + a\lambda e^{-(a+1/\lambda)\zeta}] \\ \frac{\sigma_{K\Phi}^{(2)}(\zeta)}{\sigma_Y^2 K_G q L} &= \frac{\lambda}{1 + a\lambda} [e^{-(a+1/\lambda)\zeta} - 1] \end{aligned} \quad (\text{C13})$$

$$\begin{aligned} \frac{C_{K\Phi}^{(2)}(\zeta, z)}{\sigma_Y^2 q K_G L} &= \frac{1}{1 + a\lambda} e^{-\zeta/\lambda - az} + \frac{1}{1 - a\lambda} e^{(\zeta-z)/\lambda} \\ &- \frac{2}{1 - a^2 \lambda^2} e^{a(\zeta-z)} \quad 0 \leq \zeta \leq z \end{aligned} \quad (\text{C14})$$

$$\frac{C_{K\Phi}^{(2)}(\zeta, z)}{\sigma_Y^2 q K_G L} = \frac{1}{1 + a\lambda} [e^{-\zeta/\lambda - az} - e^{(z-\zeta)/\lambda}] \quad z \leq \zeta \leq 1.$$

where $\lambda = l_y/L$. Substituting (55), (C13), and (C14) into (52) and (54) gives $f_2(\zeta)$, q_2 , $f_3(\zeta, z)$, and $q_3(\zeta)$. Substituting f_2 , h_2 , and q_2 into (C9) leads, after evaluating some quadratures, to (56). Since $f_3(z, \zeta)$ is continuous at $z = \zeta$, one can interchange the limit $\zeta \rightarrow z$ and the integration in (C9) with $i = 3$. Substituting f_3 , h_3 , and q_3 into (C9) and taking the limit as $\zeta \rightarrow z$ yields, after integration, (57).

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